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6 AUTHOR(S)
A. Luzar, A.K. Soper* and D. Chandler

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Department of Chemistry, University of California
Berkeley, CA 94720 and
*ISIS Science Division, Rutherford Appleton Laboratory,
Chilton, Didcot, Oxon OX11 0QX, United Kingdom

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by

A. Luzar, A.K. Soper* and D. Chandler

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Department of Chemistry
University of California, Berkeley
Berkeley, CA 94720

and

*ISIS Science Division, Rutherford Appleton Laboratory
Chilton, Didcot, Oxon OX11 0OX
United Kingdom

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Abstract

The structure of liquid dimethylsulphoxide (DMSO) at 25°C is explored using a combination of neutron diffraction with isotope substitution and computer simulation techniques. The potentials used in the computer simulation consist of Coulomb and 6–12 Lennard-Jones interactions for each of the carbon, oxygen and sulfur sites on the molecule. To interpret the neutron diffraction data most effectively it is necessary to refine both the molecular internal structure *and* the intermolecular contributions to the measured structure factors at the same time, in order to separate the intermolecular terms correctly, because there is a large degree of overlap between intramolecular and intermolecular distances. This renders the data far more sensitive to the intermolecular forces than if this analysis were not performed. Direct comparison of neutron diffraction data and computer simulation results indicates that existing models of the molecular force field give a sensible description of the liquid structure, although there are some discrepancies which are not fully understood at this time. The question of whether this material can be regarded as an associated liquid, as it is frequently referred to, is dicussed. All tests for association that have so far been applied to both the diffraction data and the computer simulation results do not indicate a highly ordered molecular association in the liquid.